EXTENDED COUPLED CLUSTER TECHNIQUES FOR EXCITED STATES:
APPLICATIONS TO QUASISPIN MODELS

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1. INTRODUCTION

We have described both in an earlier volume in this series and elsewhere how the so-called extended coupled cluster method (ECCM) can be used to give an extremely general microscopic description of quantum-mechanical many-body and field-theoretical systems. The formalism is in principle exact, capable of being systematically implemented at various levels of approximation, and essentially applicable to all systems governed by some underlying Schrödinger dynamics. The reader is referred to the earlier article for a full discussion of its relationships with both the earlier (normal) coupled cluster method (NCCM) or exp(S) approach of Coester and Kümmele, and the more primitive configuration-interaction (CI) method. Special attention was focussed there on the interpretation of each method within the context of time-independent perturbation theory, in terms of suitably defined generalized tree-diagram structures. Particular applications of the ECCM which have been explored in previous volumes of this series, have provided fully microscopic effective gauge-field descriptions both of a charged impurity in a polarizable medium (applicable, for example, to the important experimental tool of positron annihilation in metals), and of the zero-temperature quantum fluid dynamics of a strongly-interacting condensed Bose fluid.

We have shown elsewhere how the ECCM provides a biorthogonal formulation of the bra and ket states of an N-body system in terms of a set of quasi-local and c-number ("classical") generalized mean fields or generalized order parameters. A key feature of the method is that all of these amplitudes, which between them completely describe the full system in terms of its various n-body subsystems (n = 1,2,...,N), are linked-cluster quantities. Since they all exactly obey the cluster property, the formalism is, in principle, capable of describing such phenomena as spontaneous symmetry breaking and phase transitions. We have further demonstrated how the ECCM enables an arbitrary quantum many-body problem to be mapped exactly onto a well-defined classical Hamiltonian mechanics for these same many-body, classical, multi-local, configuration-space amplitudes, which fully parametrize the original system.

Given that the original description of the ECCM as reviewed above, was
based on a very general time-dependent formulation, it is possible to discuss
the linear response of the system in the usual way by considering small
oscillations around the (ground-state) equilibrium. In this way, we have shown
elsewhere how the collective eigenmodes may be found by thus linearizing the
equations of motion. It has furthermore been demonstrated how this formally
exact ECCM description may be viewed as an exact generalization of the
well-known random phase approximation (RPA) of Bohm and Pines. It is in this
sense that the ECCM cluster amplitudes referred to above, may be precisely
interpreted as a set of generalized multi-local mean fields acting in the
many-body configuration space. We have also shown how the stationary excited
energy-eigenstates may be described within the ECCM by analogy with their
parametrization in the NCCM due to Emrich. Finally, in the same paper it has
also been shown that there is an exact one-to-one correspondence between the
excited states so obtained as the solution to a set of linear ECCM eigenvalue
equations, and the collective eigenmodes of the effective Hamiltonian obtained
from expanding, up to second-order terms, the average-value functional for the
energy in powers of the deviations from their equilibrium values of the ECCM
cluster amplitudes.

One of our primary aims here is to introduce a new variational functional
for the excitation energies. This new formulation not only retains all of the
positive attributes of the previous versions of the ECCM, but it also provides
both a different description of the excited states and one which allows for
further flexibility in the various approximate implementations of the method
in practice.

The basic ingredients of the stationary (time-independent) version of the
(ground-state) ECCM are first briefly summarized in Sec.2. After its extension
to excited states is similarly reviewed in Sec.3, the new variational
functional for the excited states and their excitation energies is introduced
in Sec.4. As a concrete application of the method, it is tested in Sec.5 with
considerable success on the SU(2) quasispin model of Lipkin, Meshkov and
Glick, which models the spherical to deformed shape transition of atomic
nuclei at high spins, via the spontaneous breakdown of parity at high values
of the coupling parameter which characterizes the model. It is explicitly
shown how both phases are very well described by the formalism in a single
calculational scheme. Finally, the results are discussed in Sec.6.

2. ELEMENTS OF THE ECCM GROUND-STATE PARAMETRIZATION

The static ground-state ECCM has at its heart a double similarity
transformation, \( A \rightarrow \hat{A} \), for an arbitrary operator \( A \) in the Hilbert space,

\[
\hat{A} = e^{S''} e^{-S} A e^{S'} e^{-S''},
\]

(1)

which is induced by the following basic parametrizations of the exact
ground-state ket and bra energy eigenvectors,

\[
\vert \psi \rangle = e^S \vert \Phi \rangle = e^{S''} e^{-S} \vert \Phi \rangle, \quad (2a)
\]

\[
\langle \psi' \vert = \langle \Phi \vert e^{S''-S}, \quad (2b)
\]

in terms of cluster operators \( S \) and \( S'' \) and some suitable (normalized) model
state \( \vert \Phi \rangle \). This model state is often, but not necessarily, chosen to be the
appropriate non-interacting ground state in the limit where the interparticle
forces are adiabatically switched off. Equations (2a,b) clearly imply the
definite normalization, \( \langle \psi' \vert \psi \rangle = 1 \). The exact eigenstates of Eq.(2) are
assumed to be the non-degenerate ket and bra ground states of the many-body
Hamiltonian \( H \),
\[ H|\Psi\rangle = E_0|\Psi\rangle , \quad \langle\Psi'|H = E_0 \langle\Psi'| \]  

(3)

The prime in the bra-state notation introduced above is intended to remind us that although \( \langle\Psi'| = \text{const.} \times (|\Psi\rangle)\) as usual for a hermitian Hamiltonian, the parametrizations of Eq.(2) are clearly not manifestly hermitian adjoints of each other. Indeed, in subsequent truncations of the (otherwise exact) theory, this hermiticity cannot be guaranteed \textit{a priori}. The ground-state Schrödinger equations (3) are thus exactly mapped to the forms,

\[ \hat{H}|\Phi\rangle = E_0|\Phi\rangle , \quad \langle\Phi|\hat{H} = E_0 \langle\Phi| \]  

(4)

where the doubly similarity-transformed operator \( \hat{H} \) is again not manifestly hermitian, since the transformation of Eq.(1) is not unitary.

Turning to the two cluster operators defined in Eqs.(2a,b), \( S (S'') \) is defined to be constructed solely from creation (destruction) pieces with respect to the state \( |\Phi\rangle \), so that

\[ \langle\Phi|S = 0 = S''|\Phi\rangle . \]  

(5)

We note in passing that the second equation in Eq.(2a) follows from the first defining relation by making use of Eq.(5). This latter equation also implies the intermediate normalization for the ket eigenstate, \( \langle\Phi|\Psi\rangle = \langle\Phi|\Phi\rangle = 1 \).

Implicit in Eq.(5) and the statement which precedes it is that the otherwise rather free choice of model state \( |\Phi\rangle \) is made so as to fulfill the only requirement made of it, namely that the algebra of all possible operators in the many-body Hilbert space is spanned by the two Abelian subalgebras of creation and destruction operators defined with respect to \( |\Phi\rangle \). In other words, one assumes that these two subalgebras and the state \( |\Phi\rangle \) are cyclic, in the sense that an arbitrary ket (bra) state in the Hilbert space may be constructed from some suitable linear combination of states obtained from \( |\Phi\rangle \) \( (\langle\Phi'| \) by pre-multiplication (post-multiplication) with elements of the set of creation (destruction) operators.

It is thus possible to define complete orthonormal sets of creation operators \( \{C_i\} \) and their hermitian adjoint destruction counterparts \( \{C_i^\dagger\} \), where the many-body configuration space index \( i \) represents a suitable set of single-particle labels. Examples have been given elsewhere, and their choice for the LMG model used as illustration here, is made explicit in Sec.5. With respect to some suitable (generalized) Kronecker symbol \( \delta(i,j) \) in the set-indices \( i \) and \( j \), we have the orthonormality relation,

\[ \langle\Phi|C_iC_j^\dagger|\Phi\rangle = \delta(i,j) \]  

(6)

and the completeness relation for the resolution of the identity operator \( I \),

\[ I = \sum_i C_i^\dagger|\Phi\rangle\langle\Phi|C_i = |\Phi\rangle\langle\Phi| + \sum_i C_i^\dagger|\Phi\rangle\langle\Phi|C_i . \]  

(7)

The prime on the sum in Eq.(7) is used henceforth to exclude from the sum the term \( i = 0 \), where, by definition, \( C_0^\dagger = I \).

The ECCM cluster operators \( S \) and \( S'' \), defined by Eqs.(2a,b), now have the exact representations,

\[ S = \sum_i S_i C_i^\dagger , \quad S'' = \sum_i S_{i'} C_i \]  

(8)
An alternative pair of cluster operators to \(\{S, S''\}\) is denoted by \(\{\Sigma, \Sigma'\}\), and defined as follows,

\[
\Sigma = \sum_i \sigma_i \mathcal{C}_i^+ \quad \Sigma' = \sum_i \sigma'_i \mathcal{C}_i^+ ;
\]

\[
\sigma_i = \langle \Phi | \mathcal{C}_i e^{S''} S | \Phi \rangle \quad \sigma'_i = \mathcal{S}''_i .
\] (9)

One of the most important attributes of the ground-state ECCM is that both sets of \(c\)-number amplitudes \(\{S_i, S''_i\}\) and \(\{\sigma_i, \sigma'_i\}\), either one of which completely characterizes the ground-state many-body problem, are comprised of wholly-linked cluster amplitudes. Each amplitude thereby obeys the cluster property, and has a definite linked diagrammatic representation. The formalism is hence also manifestly size-extensive.

The ground-state expectation value of an arbitrary operator \(A\),

\[
\langle A \rangle = \langle A \rangle = \langle \Psi' | A | \Psi' \rangle = \langle \Phi | \hat{A} | \Phi \rangle ,
\] (10)

may thus be regarded as a functional of either complete set of amplitudes \(\{S_i, S''_i\}\) or \(\{\sigma_i, \sigma'_i\}\). In both cases, it has a well-defined linked structure.2,3

In particular, the ground-state energy functional, \(\langle H \rangle = E_0\), may be so expressed in terms of fully connected diagrams, thereby making explicit the Goldstone linked cluster theorem. We have shown1,2 that the ground-state Schrödinger equations (3) are fully equivalent to the requirement that \(\langle H \rangle\) be stationary with respect to small variations in each of the cluster amplitudes \(\{\sigma, \sigma'\}\), say,

\[
\delta\langle H \rangle / \delta \sigma_i = 0 = \delta\langle H \rangle / \delta \sigma'_i ,
\] (11)

which equations may formally be used to solve for the cluster amplitudes. Finally, it has been shown in Ref.[2] how such general matrix elements involving \(\hat{A}\) as \(\langle \Phi | \mathcal{C}_i A \mathcal{C}_j^+ | \Phi \rangle\), which are needed for the further algebraic development of the formalism, may be expressed in terms of the first- and second-order functional derivatives of the expectation value \(\langle A \rangle\) with respect to the cluster amplitudes. This relation takes the especially simple form for the Hamiltonian operator at the stationary ground-state equilibrium,

\[
\langle \mathcal{C}_i \mathcal{H} \mathcal{C}_j^+ | \Phi \rangle = E_0 \delta(i,j) + \delta^2 \langle H \rangle / \delta \sigma_i \delta \sigma_j + \sum_k \sigma_{i+k} \delta^2 \langle H \rangle / \delta \sigma_k \delta \sigma_j ,
\] (12)

for \(i \neq 0 \neq j\), in terms of second-order derivatives only, in view of Eq.(11). The cluster amplitude in Eq.(12) with the compound set-index \((i+k)\) is defined as,

\[
\sigma_{i+k} = \langle \Phi | \mathcal{C}_i \mathcal{C}_k e^{S''} S | \Phi \rangle .
\] (13)

3. ECCM DESCRIPTIONS OF THE EXCITED STATES

The corresponding excited-state Schrödinger equations,

\[
\mathcal{H} | \psi'_{\lambda} \rangle = (E_0 + \epsilon_{\lambda}^\prime) | \psi'_{\lambda} \rangle , \quad \langle \psi'_{\lambda} | \mathcal{H} = (E_0 + \epsilon_{\lambda}^\prime) \langle \psi'_{\lambda} | ,
\] (14)

may also be written in terms of the similarity-transformed Hamiltonian as,

\[
\hat{\mathcal{H}} | \chi'_{\lambda} \rangle = (E_0 + \epsilon_{\lambda}^\prime) | \chi'_{\lambda} \rangle , \quad \langle \chi'_{\lambda} | \hat{\mathcal{H}} = (E_0 + \epsilon_{\lambda}^\prime) \langle \chi'_{\lambda} |.
\] (15)
A comparison of Eqs.(14) and (15) thus implies the connections,
\[ |\psi_{\lambda}\rangle = e^{S - S''} |\lambda\rangle, \quad \langle \psi_{\lambda}' | = \langle \lambda'| e^{S''} e^{-S}. \]

Motivated by the comparable NCCM parametrization of Emrich\textsuperscript{10} for the excited ket states, we introduce the convenient parametrizations of the states \( |\lambda\rangle \) and \( \langle \lambda'| \)
\[ |\lambda\rangle = \sum_i \lambda_i \phi_i, \quad \langle \lambda'| = \sum_i \lambda_i \phi_i^* \]

in terms of excitation and de-excitation operators, \( \lambda_i \) and \( \lambda_i^* \) respectively,
\[ \lambda_i = \sum_j \lambda_i^j \phi_i^j, \quad \lambda_i^* = \sum_j \lambda_i^j \phi_i^j. \]

By combining Eqs.(4), (15) and (17), the excited-state Schrödinger equations may be written in the explicit forms,
\[ \{\hat{H}, \lambda_i\} |\phi\rangle = \varepsilon_i \lambda_i |\phi\rangle, \quad \langle \phi | [\lambda_i^*, \hat{H}] = \varepsilon_i \langle \phi | \lambda_i \]
in terms of the excitation energies \( \varepsilon_i \) directly. Projection of the former and latter of Eqs.(19) with the states \( \langle \phi | \lambda_i \) and \( \lambda_i^* |\phi\rangle \) respectively, then gives the ECCM equations for the c-number amplitudes \( \{\lambda_i\} \) and \( \{\lambda_i^*\} \) which completely characterize the excited states, as coupled sets of linear eigenvalue equations. By making use of the completeness relation (7) and Eq.(12), one may also readily rewrite these eigenvalue equations in the form,
\[ \sum_j \left( \frac{\delta^2 \langle \mathbf{H}\rangle}{\delta \sigma_j^\dagger \delta \sigma_j} + \sum_k \sigma_{j+k} \frac{\delta^2 \langle \mathbf{H}\rangle}{\delta \sigma_k \delta \sigma_j} \right) \lambda_i^j = \varepsilon_i \lambda_i^j, \quad \sum_j \lambda_i^j \left( \frac{\delta^2 \langle \mathbf{H}\rangle}{\delta \sigma_j^\dagger \delta \sigma_j} + \sum_k \sigma_{j+k} \frac{\delta^2 \langle \mathbf{H}\rangle}{\delta \sigma_k \delta \sigma_j} \right) = \varepsilon_i \lambda_i^j. \]

All of the input ground-state quantities inside the parentheses in Eqs.(20a,b) are evaluated at the stationary equilibrium found from Eq.(11).

We have also considered\textsuperscript{8} the dynamics of small oscillations of the system around this stationary point, in terms of an effective second-order Hamiltonian \( \hat{H}^{(2)} \), which is bilinear in the deviations from their equilibrium values of the cluster amplitudes \( \{\sigma_i, \sigma_i^*\} \), and which is obtained by linearizing the equations of motion. It is self-evidently found by expanding \( \hat{H} \) around the stationary equilibrium defined by Eq.(11) up to second order. It has been shown\textsuperscript{8} how the eigenfrequencies of \( \hat{H}^{(2)} \) are identical to the excitation energies \( \varepsilon_i \) found above. We have also explicitly demonstrated how this latter procedure produces an exact generalization of RPA, and hence how the ground-state amplitudes \( \{\sigma_i, \sigma_i^*\} \) may thus be viewed as a set of (multi-local) generalized mean many-body fields in the configuration space where they are now labelled by the (sets of single-particle) indices \( \{i\} \).

4. AN EXCITATION-ENERGY FUNCTIONAL

Up to this point our parametrizations of both the ground and excited many-body states have been formally exact. In practice one must, however, approximate. Perhaps the most natural such approximation scheme is the so-called SUB(n) scheme for the ground-state formalism and the SUB(m,n) scheme.
for excited states. In the SUB(n) scheme, the configuration-space indices \( \{i\} \) in either the set \( \{S_i, S'_i\} \) or \( \{\sigma_i, \tilde{\sigma}_i\} \) of cluster amplitudes, are restricted to at most \( n \) single-particle labels. Similarly in the SUB(m,n) scheme, the ground-state amplitudes are truncated at \( m \)th-order clusters as above, and at the same time the excitation amplitudes \( \{X'_i, Y'_i\} \) are similarly truncated at \( m \)th order. In both cases, the higher amplitudes are set identically to zero and the remaining truncated sets of equations are then solved, ideally without further approximation. We note that although the ground-state formalism is based on the variational principle expressed in Eq.(11), the resulting approximate values for \( E_0 \) in the SUB(n) scheme are not, in general, guaranteed to be upper bounds, since our whole formalism is a biorthogonal one, which is not manifestly hermitian at an arbitrary level of truncation.

We also note that although the NCCM, which is based upon a single similarity transformation in terms of the single cluster operator \( S \), has the distinctly advantageous attribute that at any level of truncation the ground-state equations are of finite order in the cluster amplitudes, the double similarity transformation of the ECCM spoils this property. It transpires that in order both to keep the practical applications of the ECCM as compact as possible, and to circumvent this problem as far as practicable, the ground-state parametrization is best considered in terms of the original cluster amplitudes \( \{S_i, S'_i\} \). This is in spite of the fact that the set \( \{\sigma_i, \tilde{\sigma}_i\} \) forms a much more symmetric and canonical set of coordinates for the theoretical discussions and formal applications of the method. We thus consider the ground-state energy functional \( \langle \Phi \rangle \) from Eq.(10) in the form \( E_0 = E_0[S_i, S'_i] \), where

\[
E_0[S_i, S'_i] = \langle \Phi | e^{S''} e^{-S} H e^{S} | \Phi \rangle .
\]

(21)

Stationarity of this ground-state energy functional with respect to each of the independent amplitudes \( \{S_i, S'_i\} \) leads to the set of equations which determine these amplitudes, and which are fully equivalent to the Schrödinger equations (3),

\[
\langle \Phi | e^{S''} e^{-S} [H, C_i] e^{S} | \Phi \rangle = 0 , \quad i \neq 0 ,
\]

(22a)

\[
\langle \Phi | C_i e^{S''} e^{-S} H e^{S} | \Phi \rangle = 0 , \quad i \neq 0 .
\]

(22b)

We now attempt to construct a comparable functional for the excitation energies. With this aim in mind we introduce a new excitation operator \( S^\lambda \), defined to be the creation part of the operator product \( \exp(-S'')X^\lambda \),

\[
S^\lambda | \Phi \rangle = e^{-S''} X^\lambda | \Phi \rangle , \quad S^\lambda = \sum_i S'^\lambda_i C_i .
\]

(23)

It is clear from a comparison of Eqs.(9) and (23) that the relationship between the excitation amplitudes \( S'^\lambda_i \) and \( X^\lambda_i \) is thus the precise counterpart for the excited states of that between the amplitudes \( S_i \) and \( \sigma_i \) for the ground state. Since the operators \( S \) and \( S^\lambda \) commute, we may once again combine the Schrödinger equations (3) and (14) for the ground and excited ket states respectively, to obtain the relation

\[
e^{-S''}[H, S^\lambda] e^S | \Phi \rangle = \varepsilon_{\lambda} S^\lambda | \Phi \rangle .
\]

(24)

By taking the inner product of Eq.(24) with the state \( \langle \Phi | Y^\lambda \exp(-S'') \), we
readily obtain the functional,

$$
\varepsilon_{\lambda} [S_1^\lambda, Y_1^\lambda] = \frac{\langle \Phi | Y_1^\lambda e^{-S_1^\lambda} [H, S_1^\lambda] e^{S_1} | \Phi \rangle}{\langle \Phi | Y_1^\lambda e^{-S_1^\lambda} S_1^\lambda | \Phi \rangle},
$$

(25)

for the excitation energy.

If the excitation-energy functional $\varepsilon_{\lambda}$ of Eq. (25) is now required to be stationary with respect to each of the independent amplitudes $(S_1^\lambda, Y_1^\lambda)$, we readily arrive at the generalized eigenvalue equations,

$$
\langle \Phi | Y_1^\lambda e^{-S_1^\lambda} e^{-S_1^\lambda} [H_1, C_1^\lambda] e^{S_1^\lambda} C_1^\lambda | \Phi \rangle - \varepsilon_{\lambda} \langle \Phi | Y_1^\lambda e^{-S_1^\lambda} C_1^\lambda | \Phi \rangle = 0,
\tag{26a}
$$

$$
\langle \Phi | C_1^\lambda e^{-S_1^\lambda} e^{-S_1^\lambda} [H, S_1^\lambda] e^{S_1^\lambda} S_1^\lambda | \Phi \rangle - \varepsilon_{\lambda} \langle \Phi | C_1^\lambda e^{-S_1^\lambda} S_1^\lambda | \Phi \rangle = 0,
\tag{26b}
$$

for all $i \neq 0$, which now determine these excited-state amplitudes, and which may be compared with their ground-state counterparts in Eqs. (22a,b). By making use of both the exact ground-state equations (2) and (3), and the completeness relation of Eq. (7), it is not difficult to show that the stationarity conditions of Eqs. (26a,b) are completely equivalent to the original Schrödinger equations for the excited bra and ket states. Again, this is just as expected, since the set of amplitudes $(S_1^\lambda, Y_1^\lambda)$ now gives a complete specification of the excited states in terms of the corresponding ground states. We note that the overall normalization of the excited states has never been specified. This fact is reflected in the homogeneity of the (linear) eigenvalue equations (26a,b) for the excitation amplitudes, which are thereby determined only up to an overall multiplicative constant. Finally, we remark that the replacement $\exp(S_1^\lambda) \rightarrow I$ in Eqs. (26a) and (26b) leads to two sets of equations which are themselves trivially obtained from Eqs. (4) and (24) respectively. Furthermore, these resulting equations are simply the corresponding NCCM counterparts, due respectively to Coester and Kümmler, and to Emrich.

The SUB(m,n) approximation scheme that we have outlined above is now performed in practice by solving the excited-state equations (26a,b) for the cases $i = 1, 2, ..., m$ only, and with all higher amplitudes $(S_i^\lambda, Y_i^\lambda; i > m)$ set to zero. The ground-state amplitudes $(S_1^\lambda, S_i^\lambda)$ which are needed as input to these equations are similarly taken from the SUB(n) approximation to Eqs. (22a,b). We note that the (truncated) ground-state equations (22a,b) are nonlinear in the amplitudes $(S_i^\lambda, S_i^\lambda)$, and the possibility of multiple solutions cannot be discounted. Furthermore, the excited-state equations (26a) and (26b) form decoupled sets of equations for the amplitudes $(Y_i^\lambda)$ and $(S_i^\lambda)$ respectively. The eigenvalue spectrum $\varepsilon_{\lambda}$ obtained from either set of equations is the same. Clearly, a SUB(m,n) approximation will yield estimates for $m$ excitation energies.

5. APPLICATION TO THE LMG MODEL

In the LMG model, $N$ identical fermions are distributed between two single-particle energy levels, each of which is $N$-fold degenerate, and which are separated by an energy gap of unit magnitude. The Hamiltonian is given in terms of the usual canonical fermion creation and destruction operators, $a_{p,m}^\dagger$ and $a_{p,m}$ respectively, as
\[ H = \frac{1}{2} \sum_{p,m} m a^+_p a^+_m a_p a_m + \frac{1}{2} V \sum_{p,p',m} a^+_p a^+_m a_p a_{p'-m} - a_p a_{-m}, \]  

where the index \( m = \pm 1 \) labels the two levels and the quantum number \( p = 1,2,\ldots,N \) labels single-particle states within each level. As is by now very well-known, the model is readily mapped into its spin-algebraic equivalent,

\[ H = J_z + \frac{g}{2N} (J_+^2 + J_-^2), \quad g = NV, \]  

where the quasispin operators \( J_+, J_- \) and \( J_z \), defined as

\[ J_+ = \sum_p a^+_p a_{p+1} - a_{p-1}, \quad J_- = J_+ \quad \text{and} \quad J_z = \frac{1}{2} \sum_{p,m} m a^+_p a_{p,m} a_{p,m}, \]

are readily checked to obey the usual SU(2) algebra.

The Hamiltonian of Eq. (28) is easily seen to commute with the total quasispin operator \( J^2 = J_+^2 + J_-^2 + J_z^2 \) which has eigenvalues \( j(j+1) \) as usual.

The parity operator \( \Pi = \exp(i\hbar J_z) \), and each of the \( N \) operators \( a_p \) is readily checked to obey the usual SU(2) algebra.

The excitation operators \( S^\lambda \) and \( Y^\lambda \) have the corresponding representations,

\[ S^\lambda = N \sum_{k=1}^N (iN)^{-k} S_{k^+}^\lambda S_{k^-}^\lambda \quad \text{and} \quad Y^\lambda = N \sum_{k=1}^N (iN)^{-k} Y_{k^+}^\lambda Y_{k^-}^\lambda. \]

The factors of \( N \) in Eqs. (31) and (32) have been chosen so that each term is a thermodynamically extensive operator in the large-\( N \) limit when the c-number amplitudes \( \langle S_{k^+} S_{k^-} \rangle \) and \( \langle Y_{k^+} Y_{k^-} \rangle \) are of order unity. The imaginary factors of \( i \) similarly permit us to use real values for these amplitudes.

The above choice of \( |\Phi\rangle \) as the cyclic ket vector, and the corresponding
basis \( \{ J^k_+ \phi \} \) built on it, is not however the only possible choice. While it is true that the choice of model state or cyclic vector is irrelevant for an exact calculation (i.e., a SUB(N) calculation for the ground state), the best choice of the model state for an approximate calculation at the SUB(n) level, with \( n < N \), is not a priori obvious. In particular, one knows that the LMG model undergoes a phase transition in the vicinity of some critical coupling strength \( g \rightarrow g_c \). Thus, while in the limit \( N \rightarrow \infty \), the exact ground state \( | \psi_0 \rangle \) remains qualitatively close to the perturbative ground state \( | \Phi \rangle \) for \( g < 1 \), and in particular has \( \langle J_y \rangle = 0 \), in the region \( g > 1 \) the state \( | \psi_0 \rangle \) becomes, in the same large-N limit, deformed and doubly-degenerate, with order parameter \( \langle J_y \rangle / g(2 \pi)^{1/2} / g \). This transition is perhaps most simply studied at the lowest SUB(1) level of approximation, which is identical to Hartree-Fock approximation. In a time-dependent HF calculation it is easy to show that as \( g \rightarrow g_c^H = N/(N-1) \), the frequency of the collective excitation approaches zero, thereby signalling the phase (or shape) transition. For \( g > g_c^H \), two degenerate HF solutions exist. Neither of them any longer has parity as a good quantum number. Of course, for finite values of N these two broken-symmetry solutions can communicate via quantum tunnelling through the intervening potential barrier of finite height, and hence the transition is not sharp. Although the exact ground state has even parity, the first excited state (with odd parity) becomes exponentially close to it for increasing N. Indeed for large N and large g, the lowest several states form into such closely-spaced parity doublets.

While it is thus highly suggestive on physical grounds that either one of these two degenerate broken-symmetry or deformed HF states might form a better model state or cyclic vector in the deformed region \( g > g_c^H \) than the previous symmetric solution \( | \Phi \rangle \), it is interesting to enquire whether the coupled cluster formalism can itself suggest the most appropriate starting wavefunction \( | \Phi' \rangle \). A particularly appealing argument has been discussed by Kümmel. He suggests that an appropriate optimal choice for \( | \Phi' \rangle \) is that state which maximizes the overlap \( M \) with the exact ground state,

\[
M \equiv \frac{\langle \Phi' | \psi_0 \rangle^2}{\langle \Phi' | \Phi' \rangle \langle \psi_0 | \psi_0 \rangle}.
\]

The suggestion is implemented via the Thouless theorem, which states that any Slater determinant \( | \Phi' \rangle \) in the neighbourhood of \( | \Phi \rangle \), and hence not orthogonal to it, may be written in the form \( | \Phi' \rangle = \text{const.} \times \exp(T)| \Phi \rangle \), where \( T \) is a one-body operator (i.e., one which excites Ip-1h pairs out of \( | \Phi \rangle \)). In the case of the LMG model, the appropriate choice is clearly \( T = i \gamma J_+ \), for some constant \( \gamma \). By making use of the SU(2) algebra we may then show that

\[
| \Phi' \rangle = \exp(i \alpha J_x^+)| \Phi \rangle , \quad \gamma = \tan(\frac{1}{2} \alpha) .
\]

We may thus define a new set of (unitarily transformed) quasispin operators \( K_+ , K_- \) and \( K_z \), where

\[
K_i \equiv \exp(i \alpha J_x^+ J_i \exp(-i \alpha J_x^+) ; \quad i = x,y,z ,
\]

such that \( K_- | \Phi' \rangle = 0 \).

The state \( | \Phi' \rangle \) of Eq.(34) may then be used as an alternative cyclic vector
for any value of the angle $\alpha$, and the operators $\langle S, S' \rangle$ and $\langle S^\lambda, Y^\lambda \rangle$ may be comparably expanded as in Eqs.(31) and (32) but with the replacements $|\Phi\rangle \rightarrow |\Phi'\rangle$ and $J_\pm \rightarrow K_\pm$. In particular, the HF choice is obtained by minimizing the expectation value of the Hamiltonian in the model state,

$$\langle \Phi' | H | \Phi' \rangle = -\frac{1}{4} N \left[ \cos \alpha + \frac{1}{2} g \frac{(N-1)}{N} \sin^2 \alpha \right].$$

(36)

It is trivial to show that for $g < g_{HC}^H = N/(N-1)$, the minimal value of Eq.(36) is with $\alpha = 0$, i.e. $|\Phi'\rangle \rightarrow |\Phi\rangle$, the symmetric state. Conversely, for $g > g_{HC}^H$, the two values $\alpha = \pm \cos^{-1}\left[g^{-1} N/(N-1)\right]$ give the two degenerate minima. Alternatively, a full maximum-overlap calculation would choose the value of $\alpha$ by maximizing $M$ from Eq.(33). We show examples below of numerical results obtained with both the symmetric and deformed HF solutions for the cyclic vector.

The implementation of the ECCM for the LMG model is now straightforward. The parametrizations of Eqs.(31) and (32), or the corresponding expansions in terms of $|\Phi'\rangle$ and $K_\pm$, are inserted into Eqs.(21) and (25) for the ground-state and excitation energy functionals $E_0 [S_0, S^\prime_0]$ and $\varepsilon_\lambda [S^\lambda_1, Y^\lambda_1]$ respectively. The resulting expressions are then made stationary with respect to each of their respective parameters, as already described above. We omit all details of the remaining somewhat laborious algebraic manipulations, although the interested reader may be referred to similar calculations by one of us which have been described more fully elsewhere. We prefer instead to dwell here on the results obtained at the various SUB(m,n) levels of approximation and with both symmetric (or normal) and symmetry-breaking (or deformed) model states as cyclic vectors. Some analytical results can be given in the limit $N \rightarrow \infty$. For example, if the ground-state results from a SUB(2) approximation based on the symmetric model state $|\Phi\rangle$ for all values of $g$, are inserted into a SUB(1,2) excited-state calculation, the (first) excitation energy is found to be given as,

$$\varepsilon_1 \rightarrow \begin{cases} (1-g^2)^{\frac{1}{2}} & ; g < 1 \\ [2(g^2-1)]^{\frac{3}{2}} & ; g > 1 \end{cases}$$

(37)

This result is identical to that obtained in time-dependent HF theory, and it is also exact in this large-$N$ limit.

Typical numerical results based on the symmetric model state $|\Phi\rangle$ are shown for the $N = 14$ system in Table 1 and Fig.1. The ground-state ECCM provides excellent results in both phases of the LMG model so long as the critical value $g_{HC}$ is not approached too closely. At a given SUB(n) level, an approximate critical value is determined by the point beyond which a new branch of solutions opens up in which the odd-indexed parameters $\{S_i, S^\prime_i\}$ become non-zero, to yield a parity-violating state. Even near this critical value, the method gives results which are well-behaved and still reasonably accurate. Figure 1 illustrates this behaviour and also demonstrates the lack of a sharp transition. Results for higher values of $N$ are similar. We show in Fig.2 results for a higher value of $g$ (well into the deformed region), based on the same symmetric model state. One sees that whereas the ECCM now readily obtains estimates for the average values of the very nearly degenerate low-lying parity doublets, the level-splitting can only be seen at all in a SUB(m,n) approximation with values of the truncation index $m$ close to the maximal value $N$. The other striking feature of our results in the deformed
Fig. 1. Selected ECCM excitation energies $\varepsilon_n$ (full lines) in a SUB(14,6) approximation based on the symmetric model state as cyclic vector, for the $N = 14$ system in the critical region $1 \leq g \leq 2$. The dashed lines show the corresponding exact results.

Fig. 2. Convergence properties of the six lowest ECCM excitation energies $\varepsilon_n$ (full lines) for the $N = 30$, $g = 5$ system, as a function of the truncation index $m$, in a SUB(m,6) approximation based on the symmetric model state as cyclic vector. The horizontal dashed lines show the corresponding exact results, with the four lowest parity doublets unable to be resolved.
Table 1. The excitation energies $\epsilon_n$ for the $N = 14$ system with $g = 1.0$. Columns labelled $(m,n)$ give the ECCM results in SU8(m,n) approximation, and using the normal (symmetric) model state as cyclic vector.

<table>
<thead>
<tr>
<th>$(6,6)$</th>
<th>$(7,6)$</th>
<th>$(8,6)$</th>
<th>$(9,6)$</th>
<th>$(10,6)$</th>
<th>$(11,6)$</th>
<th>$(12,6)$</th>
<th>$(13,6)$</th>
<th>$(14,6)$</th>
<th>Exact</th>
</tr>
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<tbody>
<tr>
<td>$\epsilon_1$</td>
<td>0.649</td>
<td>0.648</td>
<td>0.648</td>
<td>0.648</td>
<td>0.648</td>
<td>0.648</td>
<td>0.648</td>
<td>0.648</td>
<td>0.648</td>
</tr>
<tr>
<td>$\epsilon_2$</td>
<td>1.557</td>
<td>1.557</td>
<td>1.554</td>
<td>1.554</td>
<td>1.553</td>
<td>1.553</td>
<td>1.553</td>
<td>1.553</td>
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</tr>
<tr>
<td>$\epsilon_3$</td>
<td>2.619</td>
<td>2.587</td>
<td>2.587</td>
<td>2.579</td>
<td>2.578</td>
<td>2.578</td>
<td>2.578</td>
<td>2.578</td>
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</tr>
<tr>
<td>$\epsilon_8$</td>
<td>8.756</td>
<td>8.756</td>
<td>8.543</td>
<td>8.543</td>
<td>8.490</td>
<td>8.490</td>
<td>8.489</td>
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<tr>
<td>$\epsilon_{11}$</td>
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<td>11.982</td>
<td>11.961</td>
<td>11.961</td>
<td>11.961</td>
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<td>13.892</td>
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<td></td>
</tr>
<tr>
<td>$\epsilon_{14}$</td>
<td>14.539</td>
<td>14.540</td>
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</table>

We display in Fig.3 the accuracy of the SU8(4) results for the ground-state correlation energy, $E_c = -E_0 N$, in the region around and above the critical point, for the $N = 14$ system and for two different choices of model state as cyclic vector. The two dashed curves are both based on the symmetric model state $|\phi\rangle$. We note that for a certain range of values of $g > g_c \approx 1.6$, a second solution which is not a parity eigenstate coexists with the normal-phase solution which is a parity eigenstate. Presumably these normal-phase solutions become increasingly unstable against small perturbations as $g$ increases further into the deformed-phase region, until some upper critical value is attained beyond which they cease to exist. Figure 3 also displays as solid curves two separate branches of SU8(4) solutions based on the deformed model state $|\phi\rangle$ as cyclic vector, with the angle $\alpha$ taking the HF value. Corresponding results in various SU8(m,4) approximations for the excitation spectrum based on the more accurate of these two deformed ground-state solutions, are shown in Fig.4. We note both the similarity of the convergence to that displayed in Fig.2, and the very good quantitative agreement with exact results at the SUB(14,4) level. Typically, these results for all 14 excitation energies are accurate to a few tenths of 1%. The results change very little if the HF value for the deformation angle $\alpha$ is replaced by that from a full maximum-overlap calculation.

6. DISCUSSION

It is clear from the numerical results that the ECCM is easily capable of
Fig. 3. The error, $(1 - E_c / E_{\text{exact}}^c)$, in the SUB(4) ECCM correlation energy, $E_c = -E_0 - \frac{1}{2}N$, for the $N = 14$ system, as a function of coupling strength $g$. The two dashed (solid) curves are based on the symmetric (deformed HF) model state as cyclic vector.

Fig. 4. Convergence properties of the four lowest ECCM excitation energies $\varepsilon_n$ (full lines) for the $N = 14$, $g = 5$ system, as a function of the truncation index $m$ in a SUB(m,4) approximation based on the deformed HF model state as cyclic vector. The ground-state SUB(4) input corresponds to the upper solid curve in Fig. 3. The horizontal dashed lines show the corresponding exact results.
giving a good quantitative description of the excitation spectrum, on both sides of the shape transition, in a single calculational scheme based upon a fixed model state. In particular, this model state may either be the perturbative symmetric state or a non-perturbative symmetry-breaking deformed state. The method yields high accuracy even at relatively low SUB(m,n) levels of truncation, except for values of the coupling constant close to the critical value.

The sole qualitative feature of the spectrum that the ECCM has difficulty in describing accurately is the splitting of the nearly degenerate parity doublets in the highly deformed region. The physical reasons for this are nevertheless quite clear. Thus, by the fundamental nature of its linked-cluster construction, the ECCM is geared to a local description of the many-body system, whereas symmetry-breaking is an essentially global phenomenon. It seems intuitively clear that in order to bring these disparate features into a unification, we would need to incorporate into the ECCM some aspect of the global symmetry property from the outset. In particular, our best description of the highly deformed region has been built on a single cyclic vector, which is either one of the two degenerate deformed model states \( |\phi> \) for some choice of the angle \( \pm \alpha \). It would be of considerable interest to develop a generalized version which incorporates both on an equal footing. Such a formulation would have even wider applicability.

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